Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Electronic correlation effects in SrRuO3 ultra-thin films LIANG SI, Institute of Solid State Physics, Vienna University of Technology, ZHICHENG ZHONG, Max Planck Institute for Solid State Research, OLEG JANSON, GANG LI, JAN TOMCZAK , KARSTEN HELD, Institute of Solid State Physics, Vienna University of Technology, COMPUTATIONAL MATERIALS SCIENCE TEAM, ELECTRONIC STRUCTURE OF CORRELATED MATERIALS TEAM — SrRuO3 (SRO) is a ferromagnetic metal with an appreciably high Curie-temperature of 160 K and a ferromagnetic moment of 0.8-1.6 uB/Ru. Recent experimental studies on SRO thin films show that both electronic and magnetic ground states drastically depend on the nature of the surface. Ultra-thin (001)-oriented films are insulating and lack ferromagnetism, while in (111)-oriented films ferromagnetic moments and Tc are enhanced compared with bulk. Here we investigate SRO films by density functional theory (DFT)+U and DFT+dynamical mean-field theory (DMFT). In agreement with the experiments, we find that metallic ferromagnetism in SRO (001)-oriented films vanishes below a certain critical layer thickness. We propose a new route for tuning the properties of these thin films and show that room temperature ferromagnetism can be attained by electron doping. For the SRO (111)-oriented thin films, we find that the enhanced Tc is facilitated by electronic correlation effects and the geometric confinement. The experimentally observed enhancement of ferromagnetic moments in SRO(111)-oriented thin films is addressed by considering the stability of the high-spin Ru state in the presence of oxygen vacancies. Finally, the topological properties of SRO (111)-oriented bilayers will be discussed.

Liang Si
Vienna Univ of Technology

Date submitted: 04 Nov 2015 Electronic form version 1.4